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Molecular Hydrogen Cross Sections

Particle-In-Cell (PIC) simulation codes were shown to be a suitable tool for modeling collisional plasmas, in particular self-sustained discharges and breakdown in gases. For this purpose, they have to be coupled with a Monte Carlo Collisional (MCC) module able to model charged particle interaction with a background gas via random numbers. Molecular Hydrogen is often used as background gas in such simulations, but numerical data or interpolation formula of electron and ion impact cross section are not so easy to collect. In this short report, both interpolating formulae and tabulated data will be presented, as collected from a wide variety of literature sources.

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Abstract

Particle-In-Cell (PIC) simulation codes were shown to be a suitable tool for modeling collisional plasmas, in particular self-sustained discharges and breakdown in gases. For this purpose, they have to be coupled with a Monte Carlo Collisional (MCC) module able to model charged particle interaction with a background gas via random numbers. Molecular Hydrogen is often used as background gas in such simulations, but numerical data or interpolation formula of electron and ion impact cross section are not so easy to collect. In this short report, both interpolating formulae and tabulated data will be presented, as collected from a wide variety of literature sources.

Contents

1 Introduction

Hydrogen is a highly employed gas as industrial plasmas source in general, and in Plasma Focus discharges in particular, both for applicative use and experimental setup. In order to run microscopical simulations of Hydrogen plasmas discharges it is necessary, then, to implement H_2 cross sections databases for a Monte Carlo (MC) treatment of collisional processes [1, 2, 3].

2 Molecular Hydrogen Processes

In PIC-MCC simulations, generally, H_2 is supposed to be a uniformly distributed background neutral specie with a density n depending with time on process evolution. Electrons and ions will collide with neutral particles (not followed as simulation particles) undergoing a various set of reactions. Since the target is represented by a neutral molecule, a full set of nucleus excitation collisions adds to the electronic excitation ones. A subset of all possible reactions has been chosen by excluding every process whose cross section values never exceed 1.E-3 Å^2. The complete list of the processes considered in the present database is therefore the following:

$e + H_2 \longrightarrow e + H_2$	electron elastic scattering
$e + H_2(X^1\ \Sigma_g^+, v{=}0) \longrightarrow e + H_2^*(X^1\ \Sigma_g^+, v{=}1)$	electron impact excitation
$e + H_2(X^1\ \Sigma_g^+, v{=}0) \longrightarrow e + H_2^*(X^1\ \Sigma_g^+, v{=}2)$	electron impact excitation
$e + H_2(X^1\ \Sigma_g^+, v{=}0) \longrightarrow e + H_2^*(X^1\ \Sigma_g^+, v{=}3)$	electron impact excitation
$e + H_2(X^1\ \Sigma_g^+, J{=}0) \longrightarrow e + H_2^*(X^1\ \Sigma_g^+, J{=}2)$	electron impact excitation
$e + H_2(X^1\ \Sigma_g^+, J{=}1) \longrightarrow e + H_2^*(X^1\ \Sigma_g^+, J{=}3)$	electron impact excitation
$e + H_2(X^1\ \Sigma_g^+) \longrightarrow e + H_2^*(B^1\ \Sigma_u^+)$	electron impact excitation
$e + H_2(X^1\ \Sigma_g^+) \longrightarrow e + H_2^*(C^1\ \Pi_u)$	electron impact excitation
$e + H_2(X^1\ \Sigma_g^+) \longrightarrow e + H_2^*(E^1\ \Sigma_g^+)$	electron impact excitation
$e + H_2(X^1\ \Sigma_g^+) \longrightarrow e + H_2^*(B^{`1}\ \Sigma_u^+)$	electron impact excitation
$e + H_2(X^1\ \Sigma_g^+) \longrightarrow e + H_2^*(D^1\ \Pi_u)$	electron impact excitation
$e + H_2(X^1\ \Sigma_g^+) \longrightarrow e + H_2^*(B^{``1}\ \Sigma_u^+)$	electron impact excitation
$e + H_2(X^1\ \Sigma_g^+) \longrightarrow e + H_2^*(D^{`1}\ \Pi_u)$	electron impact excitation
$e + H_2(X^1\ \Sigma_g^+) \longrightarrow e + H_2^*(b^3\ \Sigma_u^+)$	electron impact excitation
$e + H_2(X^1\ \Sigma_g^+) \longrightarrow e + H_2^*(c^3\ \Pi_u)$	electron impact excitation
$e + H_2(X^1\ \Sigma_g^+) \longrightarrow e + H_2^*(a^3\ \Sigma_g^+)$	electron impact excitation
$e + H_2(X^1\ \Sigma_g^+) \longrightarrow e + H_2^*(d^3\ \Pi_u)$	electron impact excitation
$e + H_2(X^1\ \Sigma_g^+) \longrightarrow e + H_2^*(\text{Rydberg})$	electron impact excitation
$e + H_2 \longrightarrow H + H^-$	dissociative attachment
$e + H_2 \longrightarrow 2e + H_2^+$	ionization
$e + H_2 \longrightarrow 2e + H + H^+$	dissociative ionization

A common representation of the Hydrogen molecule energy levels is plotted in Figure 1 as a function of the internuclear distance.

Even if the dependence of excitation cross sections on both the rotational and the vibrational state of the nucleus is widely known to modify the cross sections behavior of at

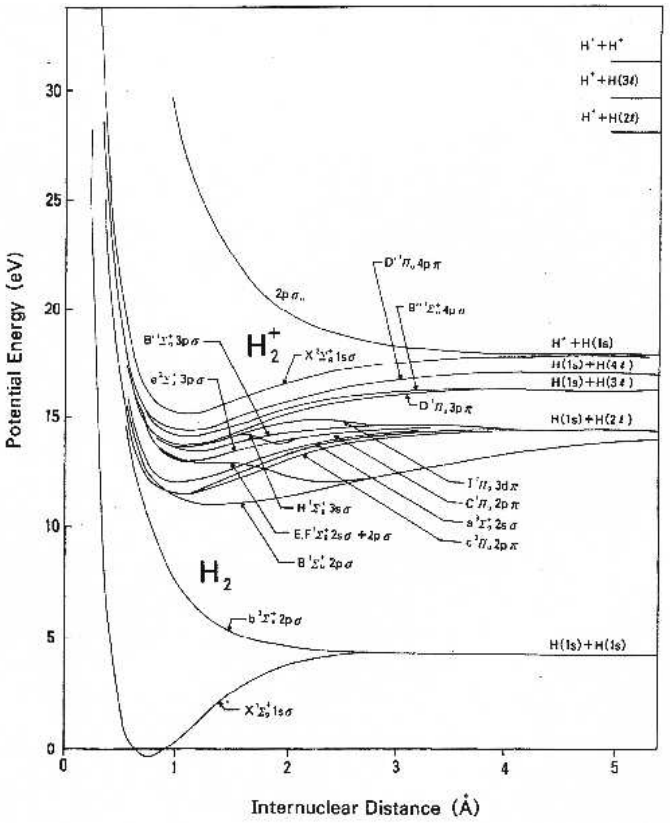

Figure 1: Electron-Hydrogen cross sections as collected in the present work.

least a factor about 3 [4, 5, 6, 7], the full roto-vibrational description of the nucleus has been neglected, since to the complexity of such a model would not correspond any significantly improvement of the MCC statistics because of the low values of the cross sections and therefore the low densities of such states. All the cross sections considered in the present work are therefore cumulative values for all vibrational and rotational initial states.

It can be also pointed out that simulation particles may collide with excited H_2 molecules, but, generally, these events are considered negligible due to the high density not-excited background particles and to the short decay time of the excited states. This assumption greatly simplify both the simulation model and the preliminary creation of the corresponding processes database.

For completion, in Appendix A all the threshold energies for the selected processes are presented.

3 Cross Section databases in literature

To create an exhaustive database of molecular Hydrogen cross sections for MC simulations several papers from literature have been investigated [4, 8, 9, 10, 11]. A complete references

collection was found in the work of Tawara *et al.* [8]: many processes are discussed and the relative references presented. All the referred papers present a finite set of point values for the cross sections, by means of which an interpolated behavior has been obtained. Unlike the Argon cross sections, for which a full set of interpolating function is easily available in literature [12], the only empirical functions for molecular Hydrogen cross sections can be found in the work of Celiberto [4], where the cross sections for the two $B^1\Sigma_u^+$ and $C^1\Pi_u$ electronic excitations and for both the dissociative attachment and ionization are given.

The first scratch of cross sections database as obtained by collecting all literature's sources is shown in Figure 2

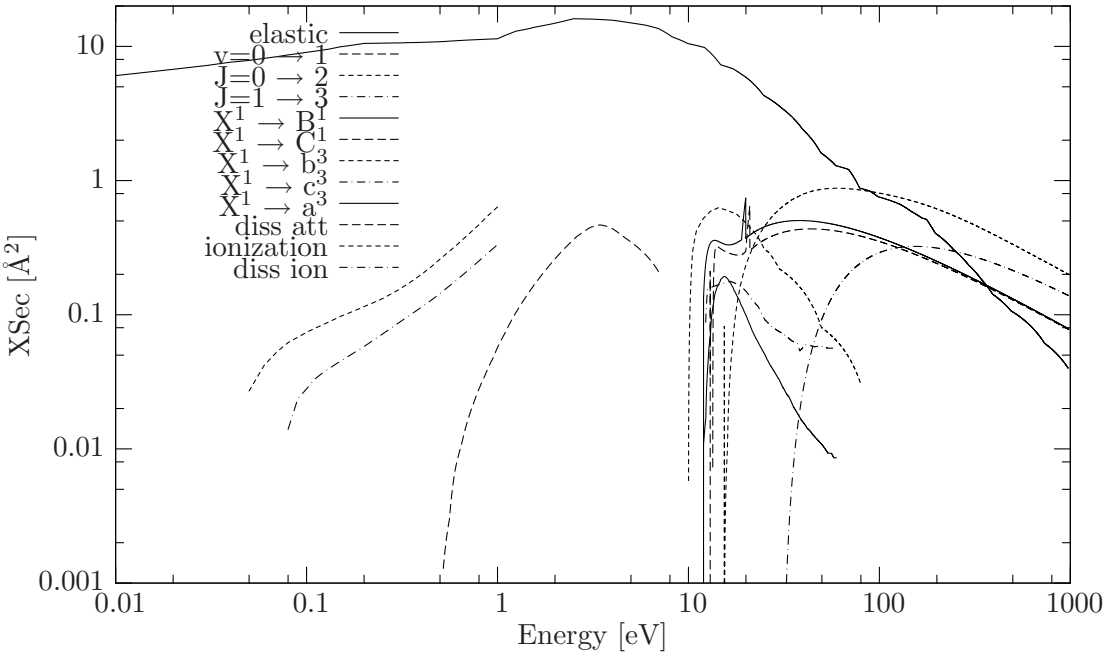

Figure 2: Electron-Hydrogen cross sections as published in literature.

An alternative database of molecular Hydrogen cross sections can be found, freely distributed, by the SIGLO software house [13]. The database is made of point values for the cross sections of the main reactions. The presented values set however is inaccurate, with too few values in high energy tails to smooth the cross sections behaviors (as shown in Figure 3).

4 The database build up

The present database has been compiled considering all the possible estimates of the cross sections values, both experimental and theoretical, collecting these data from all sources and fitting them by normalizing to the same behaviors. The resulting set of cross sections values is presented in Appendix C for the tabulated data.

As described in the work of Celiberto *et al.* [4], the two $B^1\,\Sigma_u^+$ and $C^1\,\Pi_u$ excitation

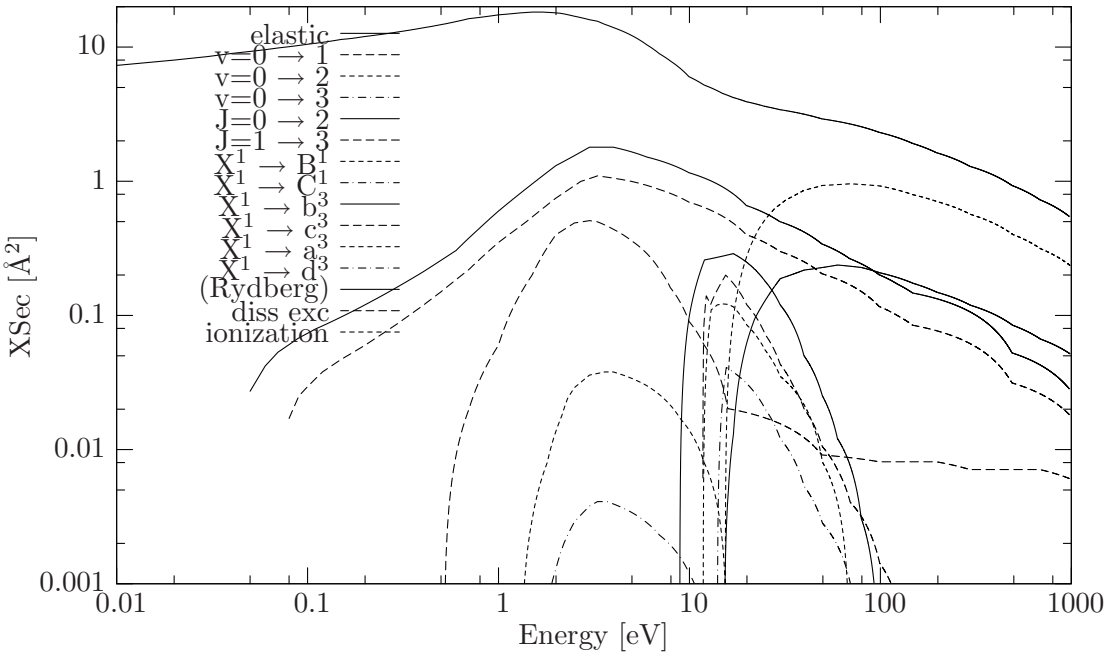

Figure 3: Electron-Hydrogen cross sections as presented in [13].

processes and both the dissociative attachment and ionization ones have been implemented into the database by means of the following interpolating functions:

- singlet electronic excitation cross sections
  - $X^1\Sigma_g^+ \rightarrow B^1\Sigma_u^+$:

$$\sigma(E) = \begin{cases} c_1^{\mathrm{B}} x_1 \mathrm{e}^{-c_2^{\mathrm{B}} x_1} + c_4^{\mathrm{B}} x_1^{c_5^{\mathrm{B}}} & \text{for } E \in [12.7, 19.0] \\ \frac{c_6^{\mathrm{B}}}{x_2} \left(\frac{x_2-1}{x_2+1}\right)^{c_{10}^{\mathrm{B}}} \left[c_7^{\mathrm{B}} + c_8^{\mathrm{B}} \left(1 - \frac{1}{2x_2}\right) \ln\left(c_9^{\mathrm{B}} + \sqrt{x_2 - 1}\right)\right] & \text{for } E \in (19.0, \infty) \end{cases} \tag{1}$$

where $x_1 = E - c_3^{\mathrm{B}}$ and $x_2 = \frac{E}{11.184}$,

- $X^1\Sigma_g^+ \rightarrow C^1\Pi_u$:

$$\sigma(E) = \begin{cases} c_1^{\mathrm{C}} x_1 \mathrm{e}^{-c_2^{\mathrm{C}} x_1} + c_4^{\mathrm{C}} x_1^{c_5^{\mathrm{C}}} + c_6^{\mathrm{C}} x_1 \mathrm{e}^{-c_7^{\mathrm{C}} x_1} & \text{for } E \in [12.4, 20.0] \\ \frac{c_8^{\mathrm{C}}}{x_2^{c_{13}^{\mathrm{C}}}} \left(\frac{x_2-1}{x_2+1}\right)^{c_{12}^{\mathrm{C}}} \left[c_9^{\mathrm{C}} + c_{10}^{\mathrm{C}} \left(1 - \frac{1}{2x_2}\right) \ln\left(c_{11}^{\mathrm{C}} + \sqrt{x_2 - 1}\right)\right] & \text{for } E \in (20.0, \infty) \end{cases} \tag{2}$$

where $x_1 = E - c_3^{\mathrm{C}}$ and $x_2 = \frac{E}{12.286}$;

- dissociative cross sections

  - attachment:

$$\sigma(E) = 1.65 \mathrm{e}^{-\frac{E-3.73}{0.45}}, \tag{3}$$

  - ionization:

$$\sigma(E) = \frac{c_1^{\mathrm{di}}}{x} \left(\frac{x-1}{x}\right)^{c_2^{\mathrm{di}}} \left(1 + c_3^{\mathrm{di}} \ln x\right) \frac{1}{30.6^{c_4^{\mathrm{di}}}} \tag{4}$$

where $x = \frac{E}{30.6}$.

In all formulae, if the energy E of the incident particle is expressed in eV the cross section σ is given in Å^2. All the fitting coefficients $c_i^{\{\mathrm{B,C,di}\}}$ are presented in Appendix D.

The resulting database, used in PIC-MCC simulations, is represented in Figure 4.

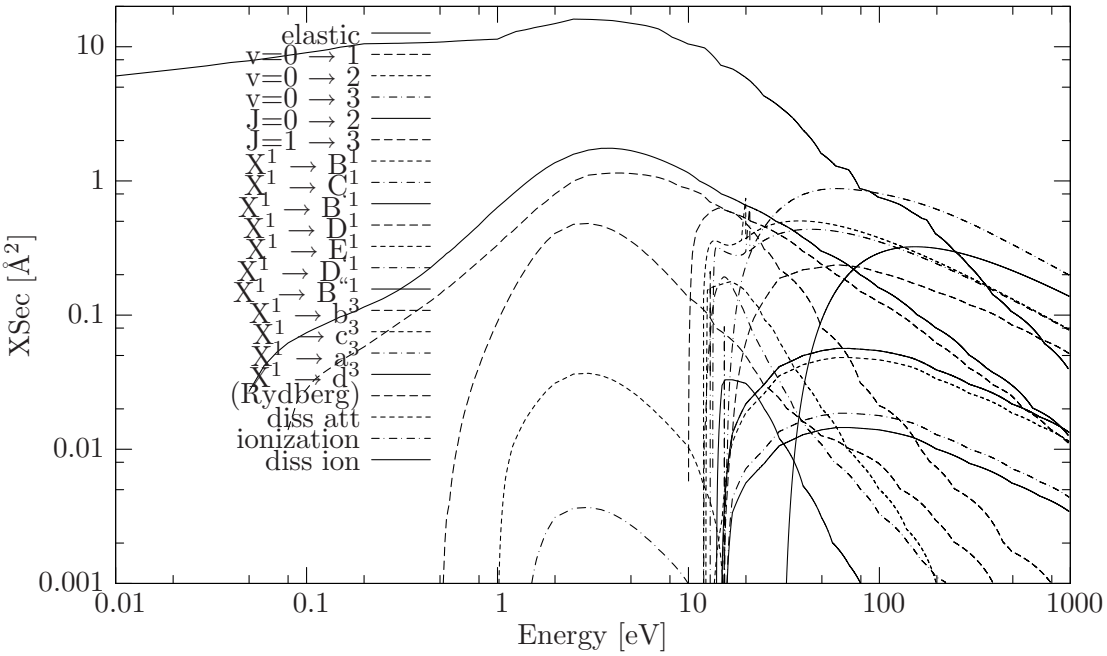

Figure 4: Electron-Hydrogen cross sections as collected in the present work.

A Excitation thresholds

Since the quantization of both the nuclear and electronic molecular energies, every exciting reaction to occur needs a projectile energy exceeding the corresponding transition energy gap. In Table 1 a list of energy thresholds is presented for the selected processes.

Process	Threshold Energy (eV)
Elastic collision	0.
Rotational excitation J=0→2	0.044
Rotational excitation J=1→3	0.073
Vibrational excitation v=0→1	0.516
Vibrational excitation v=0→2	1.000
Vibrational excitation v=0→3	1.460
Electronic excitation $B^1\,\Sigma_u^+$	12.700
Electronic excitation $C^1\,\Pi_u$	12.400
Electronic excitation $E^1\,\Sigma_g^+$	13.000
Electronic excitation $B^{`1}\,\Sigma_u^+$)	14.800
Electronic excitation $D^1\,\Pi_u$	14.900
Electronic excitation $B^{``1}\,\Sigma_u^+$	15.500
Electronic excitation $D^{`1}\,\Pi_u$	15.600
Electronic excitation $b^3\,\Sigma_u^+$	10.000
Electronic excitation $c^3\,\Pi_u$	12.300
Electronic excitation $a^3\,\Sigma_g^+$	12.000
Electronic excitation $d^3\,\Pi_u$	14.000
Electronic excitation (Rydberg)	15.200
Dissociative attachment	3.73
Ionization	15.400
Dissociative ionization	30.600

Table 1: Threshold energies for the reactions achieved into the database.

B Molecular to atomic Hydrogen dissociation

In Hydrogen plasma discharges, as in polyatomic gases in general, it is often found that new particles species are created by molecules dissociation and fragments recombination. Because of the variety of excited states (both nuclear and electronic), it is found that many collisions effect is to destabilize the molecule, leading to its indirect dissociation, which can be accompanied by photons emission.

The Hydrogen molecule is the most unstable, due to the low shielding effect of electrons to the electrostatic repulsion of the two protons in the nucleus. A wide set of colliding processes causes then the Hydrogen molecule dissociation both by direct excitation of the molecule into the "forbidden" levels (two steps dissociation) and by indirect excitation of the molecule to states whose de-excitation lead to the same forbidden levels themselves (three steps dissociation). The latter processes are therefore coupled with the emission of photons proper of the de-excitation inter-levels gap.

In Table 2 the indirect dissociation processes are presented among all the reactions considered within the database. For each one a branching ratio is given, representing the probability of the excited state to dissociate rather than decay into a lower level. For non-forbidden levels it represents the de-excitation probability to decay into a forbidden level among all possible de-excitations processes.

Process	Branching ratio
$H_2^*(b^3\Sigma_u^+) \longrightarrow H(1s) + H(1s)$	$\chi = 1.000$
$H_2^*(c^3\Pi_u) \longrightarrow H(1s) + H(1s) + h\nu$	$\chi = 1.000$
$H_2^*(a^3\Sigma_g^+) \longrightarrow H(1s) + H(1s) + h\nu$	$\chi = 1.000$
$H_2^*(d^3\Pi_u) \longrightarrow H(1s) + H^*(2l)$	$\chi = 0.298$
$H_2^*(B^{"1}\Sigma_u^+) \longrightarrow H(1s) + H^*(2l)$	$\chi = 0.967$
$H_2^*(D^{'1}\Pi_u) \longrightarrow H(1s) + H^*(2l)$	$\chi = 1.000$

Table 2: Dissociation branching ratios for the indirect dissociative reactions achieved into the database.

C Tabulated Cross Sections

Process:	Elastic	Ionization
Energy [eV]	Cross Section [Å^2]	
0.000	5.800D+000	
0.010	6.060D+000	
0.020	6.750D+000	
0.030	7.210D+000	
0.040	7.630D+000	
0.046	7.730D+000	
0.050	7.860D+000	
0.060	8.140D+000	
0.070	8.390D+000	
0.080	8.640D+000	
0.090	8.840D+000	
0.100	9.040D+000	
0.130	9.530D+000	
0.150	9.930D+000	
0.200	1.053D+001	
0.300	1.062D+001	
0.400	1.072D+001	
0.500	1.084D+001	
0.600	1.102D+001	
0.700	1.116D+001	
0.900	1.134D+001	
1.000	1.140D+001	
1.100	1.210D+001	
1.250	1.300D+001	
1.400	1.340D+001	
1.500	1.370D+001	
1.560	1.390D+001	
1.600	1.400D+001	
1.800	1.445D+001	
2.000	1.490D+001	
2.500	1.610D+001	
3.124	1.600D+001	
4.000	1.570D+001	
5.000	1.500D+001	
6.000	1.440D+001	
7.000	1.360D+001	
8.250	1.180D+001	
10.000	1.050D+001	
12.250	9.800D+000	
14.874	7.280D+000	
15.430		0.00D+000
16.000		0.10D-001
17.000		0.59D-001
17.250	6.800D+000	
18.000		1.22D-001
18.874	6.270D+000	
19.000		1.81D-001
20.000		2.35D-001
21.000	5.620D+000	
22.500		3.55D-001
25.000	4.300D+000	4.57D-001
27.500		5.44D-001
30.000		6.17D-001
31.250	3.440D+000	

Process:	Elastic	Ionization
Energy [eV]	Cross Section [Å^2]	
32.500		6.76D-001
35.000		7.28D-001
40.000	2.410D+000	8.01D-001
45.000		8.46D-001
50.000	1.600D+000	8.71D-001
55.000		8.83D-001
60.000	1.280D+000	8.86D-001
65.000		8.84D-001
70.000	1.200D+000	8.77D-001
75.000		8.69D-001
80.000	8.700D-001	8.59D-001
85.000		8.49D-001
90.000	8.300D-001	8.38D-001
95.000		8.27D-001
100.000	7.500D-001	8.16D-001
105.000		8.05D-001
110.000	7.200D-001	7.94D-001
115.000		7.84D-001
120.000	6.900D-001	7.73D-001
125.000		7.63D-001
130.000	6.600D-001	7.52D-001
135.000		7.42D-001
140.000	6.200D-001	7.32D-001
145.000		7.22D-001
150.000	5.800D-001	7.13D-001
155.000		7.03D-001
160.000	5.500D-001	6.94D-001
165.000		6.84D-001
170.000	5.200D-001	6.75D-001
175.000		6.66D-001
180.000	5.070D-001	6.57D-001
190.000	4.500D-001	6.40D-001
200.000	4.000D-001	6.23D-001
225.000		5.84D-001
250.000	3.000D-001	5.49D-001
275.000		5.17D-001
300.000	2.300D-001	4.89D-001
350.000	1.800D-001	4.40D-001
400.000	1.400D-001	4.00D-001
408.000		3.95D-001
450.000		3.67D-001
500.000	1.050D-001	3.40D-001
545.000		3.19D-001
550.000		3.16D-001
600.000		2.96D-001
650.000		2.79D-001
700.000		2.63D-001
750.000	6.010D-002	2.50D-001
800.000		2.38D-001
817.000		2.34D-001
850.000		2.27D-001
900.000		2.17D-001
950.000		2.08D-001
1000.00	3.900D-002	2.00D-001

Process:	Vibrational			Rotational	
	v= 0 → 1	v= 0 → 2	v= 0 → 3	J= 0 → 2	J= 1 → 3
Energy [eV]	Cross Section [Å^2]				
0.044				0.000D+000	
0.047				0.0185D+000	
0.050				0.027D+000	
0.055				0.035D+000	
0.060				0.042D+000	
0.065				0.048D+000	
0.070				0.053D+000	
0.073					0.000D+000
0.075					0.007D+000
0.080				0.062D+000	0.014D+000
0.085					0.0198D+000
0.090				0.068D+000	0.0237D+000
0.095					0.0265D+000
0.100				0.074D+000	0.0280D+000
0.110				0.079D+000	0.033D+000
0.120					0.0364D+000

0.130				0.088D+000	0.0394D+000
0.150				0.097D+000	0.045D+000
0.160				0.100D+000	0.048D+000
0.180				0.107D+000	0.053D+000
0.200				0.115D+000	0.058D+000
0.250				0.132D+000	0.0719D+000
0.300				0.152D+000	0.086D+000
0.350				0.175D+000	0.100D+000
0.400				0.200D+000	0.114D+000
0.450				0.228D+000	0.1285D+000
0.500				0.260D+000	0.1439D+000
0.516	0.000D+000				
0.520	0.001D+000			0.272D+000	0.1515D+000
0.540	0.003D+000			0.287D+000	0.159D+000
0.560	0.004D+000			0.297D+000	0.163D+000
0.600				0.323D+000	0.1776D+000
0.620	0.011D+000			0.338D+000	0.184D+000
0.700	0.023D+000			0.394D+000	0.2135D+000
0.800	0.041D+000			0.469D+000	0.2518D+000
0.900	0.063D+000			0.555D+000	0.2919D+000
1.000	0.089D+000	0.000D+000		0.636D+000	0.333D+000
1.100	0.118D+000	0.060D-001		0.714D+000	0.382D+000
1.200	0.150D+000	0.105D-001		0.796D+000	0.421D+000
1.400	0.218D+000	0.167D-001		0.958D+000	0.518D+000
1.460			0.000D+000		
1.500	0.254D+000	0.194D-001	0.094D-002	1.036D+000	0.569D+000
1.600	0.289D+000	0.221D-001	0.151D-002	1.112D+000	0.620D+000
1.800	0.354D+000	0.271D-001	0.241D-002	1.250D+000	0.704D+000
2.000	0.407D+000	0.311D-001	0.311D-002	1.370D+000	0.800D+000
2.500	0.476D+000	0.364D-001	0.364D-002	1.585D+000	1.000D+000
3.000	0.483D+000	0.369D-001	0.369D-002	1.704D+000	1.108D+000
3.500	0.464D+000	0.355D-001	0.355D-002	1.755D+000	1.134D+000
4.000	0.432D+000	0.330D-001	0.330D-002	1.758D+000	1.150D+000
4.500	0.394D+000	0.301D-001	0.301D-002	1.732D+000	1.149D+000
5.000	0.356D+000	0.272D-001	0.272D-002	1.689D+000	1.140D+000
6.000	0.288D+000	0.220D-001	0.220D-002	1.579D+000	1.110D+000
7.000	0.234D+000	0.179D-001	0.179D-002	1.461D+000	1.065D+000
8.000	0.193D+000	0.148D-001	0.148D-002	1.349D+000	1.000D+000
9.000	0.161D+000	0.123D-001	0.123D-002	1.247D+000	0.916D+000
10.000	0.136D+000	0.104D-001	0.100D-002	1.156D+000	0.880D+000
11.500				1.000D+000	
11.800					0.800D+000
12.000		0.550D-002			
12.800	0.100D+000				
13.000					0.700D+000
14.000	0.800D-001				
15.000				0.800D+000	
16.000		0.000D+000			0.600D+000
20.000	0.500D-001			0.660D+000	0.530D+000
21.500					0.500D+000
22.000	0.400D-001				
25.000	0.300D-001				
29.000				0.500D+000	
30.000	0.240D-001			0.490D+000	0.400D+000
33.000	0.200D-001				
40.000	0.160D-001			0.380D+000	0.300D+000
43.000	0.150D-001				
50.000	0.125D-001			0.300D+000	0.240D+000
60.000	0.115D-001				0.200D+000
70.000	0.100D-001				
80.000	0.930D-002			0.200D+000	
100.000	0.780D-002			0.160D+000	0.125D+000
130.000	0.500D-002				1.000D-001
133.000				0.125D+000	
160.000				1.000D-001	0.800D-001
165.000	0.400D-002				
200.000	0.292D-002			0.800D-001	0.620D-001
250.000	0.200D-002				0.500D-001
300.000				0.500D-001	0.400D-001
370.000				0.400D-001	
400.000	0.100D-002			0.370D-001	0.300D-001
500.000				0.300D-001	0.250D-001
575.000					0.200D-001
650.000				0.200D-001	
800.000				0.170D-001	0.140D-001
1000.000	0.100D-003		0.100D-006	0.125D-001	0.110D-001

Process:	$X^1\Sigma_g^+ \rightarrow B'^1\Sigma_u^+$	$X^1\Sigma_g^+ \rightarrow D^1\Pi_u$	$X^1\Sigma_g^+ \rightarrow E^1\Sigma_g^+$	$X^1\Sigma_g^+ \rightarrow D'^1\Pi_u$	$X^1\Sigma_g^+ \rightarrow B''^1\Sigma_u^+$	$X^1\Sigma_g^+ \rightarrow$ (Rydberg)
Energy [eV]	Cross Section [Å^2]					
13.000			0.000D+000			
14.800	0.000D+000					
14.900		0.000D+000				
15.000			3.000D-003			
15.200						0.000D+000
15.500					0.000D+000	
15.600				0.000D+000		
16.000						5.000D-003
17.000	1.300D-002	1.300D-002	1.100D-002	4.000D-003	3.000D-003	1.300D-002
18.000						3.000D-002
20.000	2.200D-002	2.200D-002	1.900D-002	7.000D-003	6.000D-003	6.300D-002
22.000						9.500D-002
25.000	3.100D-002	3.100D-002	2.600D-002	1.000D-002	8.000D-003	
30.000	4.200D-002	4.200D-002	3.600D-002	1.400D-002	1.100D-002	1.900D-001
35.000	4.600D-002	4.600D-002	3.900D-002	1.500D-002	1.200D-002	
40.000	5.000D-002	5.000D-002	4.300D-002	1.700D-002	1.300D-002	2.200D-001
50.000	5.500D-002	5.500D-002	4.700D-002	1.800D-002	1.400D-002	
60.000	5.700D-002	5.700D-002	4.900D-002	1.900D-002	1.500D-002	2.400D-001
70.000	5.700D-002	5.700D-002	4.900D-002	1.900D-002	1.500D-002	
80.000						2.300D-001
100.000	5.500D-002	5.500D-002	4.700D-002	1.800D-002	1.400D-002	2.100D-001
150.000	4.800D-002	4.800D-002	4.100D-002	1.600D-002	1.200D-002	1.750D-001
200.000	3.900D-002	3.900D-002	3.400D-002	1.300D-002	1.000D-002	1.500D-001
300.000	3.100D-002	3.100D-002	2.600D-002	1.000D-002	8.000D-003	1.200D-001
500.000	2.200D-002	2.200D-002	1.900D-002	7.000D-003	6.000D-003	8.500D-002
700.000	1.800D-002	1.800D-002	1.500D-002	6.000D-003	5.000D-003	6.700D-002
1000.000	1.300D-002	1.300D-002	1.100D-002	4.000D-003	3.000D-003	5.200D-002

Process:	$X^1\Sigma_g^+ \rightarrow b^3\Sigma_u^+$	$X^1\Sigma_g^+ \rightarrow c^3\Pi_u$	$X^1\Sigma_g^+ \rightarrow a^3\Sigma_g^+$	$X^1\Sigma_g^+ \rightarrow d^3\Pi_u$
Energy [eV]	Cross Section [Å^2]			
10.000	0.000D+000			
10.500	2.900D-001			
11.000	4.200D-001			
12.000	5.250D-001		0.000D+000	
12.019			0.007D-001	
12.042			0.021D-001	
12.065			0.050D-001	
12.077			0.085D-001	
12.100			0.127D-001	
12.300		0.000D+000		
12.330			0.170D-001	
12.347		0.119D-002		
12.430		2.060D-002		
12.450			0.283D-001	
12.509		8.030D-002		
12.570		1.537D-001		
12.600	5.600D-001			
12.680			0.453D-001	
12.800			0.559D-001	
13.000	5.900D-001			
13.030			0.701D-001	
13.150			0.871D-001	
13.260			1.013D-001	
13.380			1.098D-001	
13.410		1.621D-001		
13.500			1.183D-001	
13.610			1.282D-001	
13.730			1.409D-001	
13.960			1.523D-001	
14.000				0.000D+000
14.190			1.629D-001	
14.310			1.671D-001	
14.400	6.300D-001			
14.660			1.771D-001	
14.770			1.841D-001	
15.000				3.000D-002
15.120			1.898D-001	
15.240			1.926D-001	
15.470			1.933D-001	
15.590			1.926D-001	
15.600				3.300D-002
15.660		1.738D-001		
15.820			1.898D-001	
16.000	6.000D-001			
16.170			1.834D-001	
16.400			1.778D-001	
16.630		1.775D-001		
16.750			1.693D-001	

17.000	5.800D-001			3.300D-002
17.100			1.608D-001	
17.330			1.530D-001	
17.390		1.731D-001		
17.680			1.452D-001	
18.000	5.600D-001			
18.150			1.346D-001	
18.490			1.289D-001	
18.620		1.641D-001		
18.840			1.197D-001	
19.000	5.200D-001			
19.420			1.098D-001	
19.540		1.554D-001		
19.660			1.048D-001	
20.000			0.999D-001	3.100D-002
20.270		1.469D-001		
20.470			0.921D-001	
21.000	4.500D-001			
21.050			0.836D-001	
21.340		1.323D-001		
21.630			0.758D-001	
22.170		1.235D-001		
22.450			0.680D-001	
23.000	3.850D-001			
23.200		1.154D-001		
23.610			0.595D-001	
24.270		1.011D-001		
24.540			0.538D-001	
25.000	3.100D-001			2.000D-002
25.160		9.170D-002		
25.350			0.496D-001	
25.820			0.467D-001	
26.500	2.900D-001			
26.750			0.425D-001	
27.500		8.000D-002		
27.790			0.390D-001	
28.000	2.600D-001			
29.190			0.347D-001	
30.000	2.200D-001	6.300D-002	0.326D-001	1.200D-002
31.160			0.290D-001	
31.860			0.276D-001	
32.790			0.255D-001	
33.000		5.000D-002		
33.840			0.241D-001	
35.580			0.205D-001	
36.000		4.000D-002		
36.740			0.191D-001	
37.900			0.177D-001	
39.180			0.163D-001	
40.000		3.300D-002		5.300D-003
41.160			0.149D-001	
41.500		3.000D-002		
41.970			0.142D-001	
43.600			0.135D-001	
44.990			0.127D-001	
46.620			0.120D-001	
48.480			0.113D-001	
50.000	8.000D-002	2.000D-002		3.080D-003
50.570			0.106D-001	
52.320			0.990D-002	
54.180			0.920D-002	
57.000				2.000D-003
58.130			0.800D-002	
68.000		1.000D-002		
70.000				1.350D-003
80.000	3.100D-002	7.750D-003	0.500D-002	1.000D-003
100.000	2.100D-002	5.000D-003	0.330D-002	4.000D-004
108.000	2.000D-002		0.300D-002	
140.000		2.500D-003		
142.000			0.200D-002	
150.000				0.000D+000
165.000	1.000D-002		0.150D-002	
185.000	8.000D-003			
200.000	7.300D-003	1.000D-003	0.110D-002	
225.000			1.000D-003	
250.000	5.000D-003			
450.000	2.000D-003			
500.000	1.700D-003			
800.000	1.000D-003			
1000.000	8.000D-004	1.000D-005	0.200D-003	

D Interpolating formulae fitting coefficients

The fitting coefficient for the cross sections interpolating formulae as presented in [4] are collected in Table 5.

Coefficient	Process		
	Electronic excitation $B^1\,\Sigma_u^+$	Electronic excitation $C^1\,\Pi_u$	Dissociative Ionization
c_1	0.42566	-21.104	2.0013E4
c_2	0.77443	7.5183	2.63323
c_3	11.779	12.982	0.57363
c_4	0.12348	0.33278	2.18
c_5	0.52783	-0.12174	
c_6	1.3204	0.15650E-4	
c_7	-0.41817	-0.82171	
c_8	2.4241	1.2634	
c_9	1.5734	0.53604	
c_{10}	0.65554	1.7887	
c_{11}		0.91350	
c_{12}		0.84579	
c_{13}		0.97791	

Table 5: Fitting coefficients for equations 1, 2 and 4.

References

[1] C. K. Birdsall and A. B. Langdon. *Plasma Physics via computer simulation*. McGraw-Hill, 1976.

[2] C. K. Birdsall. Particle-In-Cell charged-particle simulations, plus Monte Carlo Collisions with neutral atoms, PIC-MCC. *IEEE Trans. on Plasma Sci.*, 19:65–85, 1991.

[3] V. Vahedi and M. Surendra. A Monte Carlo collision model for the Particle-In-Cell method: applications to argon and oxygen discharges. *Comp. Phys. Comm.*, 87:178–98, 1995.

[4] R. Celiberto *et al.* Cross sections data for electron-impact inelastic processes of vibrationally excited molecules of hydrogen and its isotopes. *At. Data and Nucl. Data Tab.*, 77(2):161–213, 2001.

[5] I. I. Fabrikant, J. M. Wadehra and Y. Xu. Resonance processes in e-H_2 collisions: dissociative attachment and dissociation from vibrationally and rotationally excited states. *Phys. Scrip.*, T96:45–51, 2002.

[6] J. N. Bardsley and J. M. Wadehra. Dissociative attachment and vibrational excitation in low-energy collisions of electrons with H_2 and D_2. *Phys. Rev A*, 20(4):1398–405, 1979.

[7] D. E. Atems and J. M. Wadehra. Nonlocal effects in dissociative electron attachment to H_2. *Phys. Rev. A*, 42(9):5201–7, 1990.

[8] H. Tawara *et al.* Cross sections and related data for electron collisions with hydrogen molecules and molecular ions. *J. Phys. Chem. Ref. Data*, 19(3):617–36, 1990.

[9] M. J. Brunger and S. J. Buckman. Electronmolecule scattering cross-sections. I. Experimental techniques and data for diatomic molecules. *Phys. Rep.*, 357:215–458, 2002.

[10] J. Tennyson and C. S. Trevisan. Low energy elecron collisions with molecular hydrogen. *Contrib. Plas. Phys.*, 42(6–7):573–7, 2002.

[11] C. F. Barnett. *The ORNL CFADC "Redbooks"*. http://www-cfadc.phy.ornl.gov/redbooks/redbooks.html, 1990.

[12] M. Frignani and G. Grasso. Argon cross sections for PIC-MCC codes. Technical Report LIN-R01.2006, LIN, 2006.

[13] *The SIGLO database*. http://www.siglo-kinema.com.